

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.25

Global applicability domain: Inside

Local applicability domain index: 4.77e-01

Confidence level: 5.52e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Dichlorvos</div> <div>Measured: 1.43</div> <div>Predicted: 1.25</div>	<div>Image not found</div> <div>Tris(2-chloroethyl) phosphate</div> <div>Measured: 1.44</div> <div>Predicted: 1.58</div>	<div>Image not found</div> <div>Heptenophos</div> <div>Measured: 2.32</div> <div>Predicted: 2.25</div>
<div>Image not found</div> <div>Busulfan</div> <div>Measured: -0.520</div> <div>Predicted: -0.282</div>	<div>Image not found</div> <div>Dimethyl (2-oxopropyl)phosphonate</div> <div>Measured: -0.860</div> <div>Predicted: -0.611</div>	